

Furan-2-carboxamide, N-butyl-N-hexadecyl-

Inchi: InChI=1S/C25H45NO2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-22-26(21-6-4-2)25(27)
InchiKey: PUTSHLIOHLMBKS-UHFFFAOYSA-N
Formula: C25H45NO2
SMILES: CCCCCCCCCCCCCCN(CCCC)C(=O)c1ccco1
Mol. weight [g/mol]: 391.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.88		Crippen Method
logp	8.003		Crippen Method
mcvol	361.070	ml/mol	McGowan Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415654&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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